U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-292 271

Guideline for the Interpretation of Ozone Air Quality Standards

(U.S.) Environmental Protection Agency, Research Triangle Park, NC

Jan 79

PB 292271

United States
Environmental Protection
Agency

Office of Air Quality
Planning and Standards
Research Triangle Park NC 27711

EPA-450/4-79-003
OAQPS No. 1.2-108
January 1979

Air

EPA

Guideline Series

Guideline for the Interpretation of Ozone Air Quality Standards

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NATIONAL TECHNICAL
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U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA 450/4-79-003	2.	3. RECIPIENT'S ACCESSION NO. PB292271
4. TITLE AND SUBTITLE Guideline for the Interpretation of Ozone Air Quality Standards		5. REPORT DATE January, 1979 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Thomas C. Curran, Ph.D		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air, Noise and Radiation Office of Air Quality Planning and Standards Research Triangle Park, North Carolina 27711		10. PROGRAM ELEMENT NO. 11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Same as box 9		13. TYPE OF REPORT AND PERIOD COVERED 14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES
Special mention should be made of the contributions of William M. Cox, Thomas B. Feagans, William F. Hunt, Jr. and Sherry L. Olson

16. ABSTRACT

This document discusses the interpretation of the National Ambient Air Quality Standards (NAAQS) for ozone that were promulgated by the U.S. Environmental Protection Agency in 1979. These standards differ from previous NAAQS in that attainment decisions are based upon the expected number of days per year above the level of the standard. The data analysis implications of this statistical formulation of an air quality standard are presented for both compliance assessment and design value estimation purposes. Example calculations are included.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution Standards Design Values Ozone		

18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS *(This Report)* Unclassified 20. SECURITY CLASS *(This page)* Unclassified	21. NO. OF PAGES 41 22. PRICE A03-A01

EPA Form 2220-1 (9-73)

EPA-450/4-79-003

OAQPS No. 1.2-108

Guideline for the Interpretation of Ozone Air Quality Standards

Monitoring and Data Analysis Division

Prepared for

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air, Noise, and Radiation
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

January 1979

OAQPS GUIDELINE SERIES

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Publication No. EPA-450/4-79-003
(OAQPS No. 1.2-108

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1. INTRODUCTION

The ozone National Ambient Air Quality Standards (NAAQS) contain the phrase "expected number of days per calendar year." [1] This differs from the previous NAAQS for photochemical oxidants which simply state a particular concentration "not to be exceeded more than once per year." [2] The data analysis procedures to be used in computing the expected number are specified in Appendix H to the ozone standard. The purpose of this document is to amplify the discussions contained in Appendix H dealing with compliance assessment and to indicate the data analysis procedures necessary to determine appropriate design values for use in developing control strategies. Where possible, the approaches discussed here are conceptually similar to the procedures presented in the earlier "Guideline for Interpreting Air Quality Data With Respect to the Standards" (OAQPS 1.2-008, revised February, 1977). [3] However, the form of the ozone standards necessitates certain modifications in two general areas: (1) accounting for less than complete sampling and (2) incorporating data from more than one year.

Although the interpretation of the proposed standards may initially appear complicated, the basic principle is relatively straightforward. In general, the average number of days per year above the level of the standard must be less than or equal to 1. In its simplest form, the number of exceedances each year would be recorded and then averaged over the past three years to determine if this average is less than or equal to 1. Most of the complications that arise are consequences of accounting for incomplete sampling or changes in emissions.

Throughout the following discussion certain points are assumed that are consistent with previous guidance [3] but should be reiterated here for completeness. The terms hour and day (daily) are interpreted respectively as clock hour and calendar day. Air quality data are examined on a site by site basis and each individual site must meet the standard. In general, data from several different sites are not combined or averaged when performing these analyses. These points are

discussed in more detail elsewhere. [3]

This document is organized so that the remainder of this introductory section presents the background of the problem, terminology, and certain basic premises that were used in developing this guidance. This is followed by a section which examines methods for determining appropriate design values. The final section discusses approaches that might be employed in cases without ambient monitoring data. This last section is brief and fairly general, because it treats an aspect of the problem which would be expected to rapidly evolve once these new forms of the NAAQS become established. In several parts of this document the material is developed in a conversational format in order to highlight certain points.

1.1. Background

The previous National Ambient Air Quality Standard (NAAQS) for oxidant stated that no more than one hourly value per year should exceed 160 micrograms per cubic meter (.08ppm). [2] With this type of standard, the second highest value for the year becomes the decision-making value. If it is above 160 micrograms per cubic meter then the standard was exceeded. This would initially appear to be an ideal type of standard. The wording is simple and the interpretation is obvious-or is it? Suppose the second highest value for the year is less than 160 micrograms per cubic meter and the question asked is, "Does this site meet the standard?" An experienced air pollution analyst would almost automatically first ask, "How many observations were there?" This response reflects the obvious fact that the second highest measured value can depend upon how many measurements were made in the year. Carried to the absurd, if only one measurement is made for the year, it is impossible to exceed this type of standard. Obviously, this extreme case could be remedied by requiring some minimum number of measurements per year. However, the basic point is that the probability of detecting a violation would still be expected to increase as the number of samples increased from the specified minimum to the maximum possible number of observations per year. Therefore, the present wording of this type of standard inherently penalizes an area that performs

more than the minimum acceptable amount of monitoring. Furthermore, the specification of a minimum data completeness criterion still does not solve the problem of what to do with those data sets that fail to meet this criterion.

A second problem with the current wording of the standard is not as obvious but becomes more apparent when considering what is involved in maintaining the standard year after year. For example, suppose an area meets the standard in the sense that only one value for the year is above 160 micrograms per cubic meter. Because of the variability associated with air quality data, the fact that one value is above the standard level means that there is a chance that two values could be above this standard level the next year even though there is no change in emissions. In other words, any area with emissions and meteorology that can produce one oxidant value above the standard has a definite risk of sometime having at least two such values occurring in the same year and thereby violating the standard. This situation may be viewed as analogous to the "10 year flood" and "100 year flood" concepts used in hydrology; i.e., high values may occur in the future but the likelihood of such events is relatively low. However, with respect to air pollution any rare violation poses distinct practical problems. From a control agency viewpoint, the question arises as to what should be done about such a violation if it is highly unlikely to reoccur in the next few years. If the decision is made to ignore such a violation then the obvious implication is that the standard can occasionally be ignored. This is not only undesirable but produces a state of ambiguity that must be resolved to intelligently assess the risk of violating the standard. In other words, some quantification is needed to describe what it means to maintain the standard year after year in view of the variation associated with air quality data. The wording of the ozone standard is intended to alleviate these problems.

1.2. Terminology

The term 'daily maximum value' refers to the maximum hourly ozone value for a day. As defined in Appendix H, a valid daily maximum means that at least

75% of the hourly values from 9:01 A.M. to 9:00 P.M. (LST) were measured or at least one hourly value exceeded the level of the standard. This criterion is intended to reflect adequate monitoring of the daylight hours while allowing time for routine instrument maintenance. The criterion also ensures that high hourly values are not omitted merely because too few values were measured. It should be noted that this is intended as a minimal criterion for completeness and not as a recommended monitoring schedule.

A final point worth noting concerns terminology. The term "exceedance" is used throughout this document to describe a daily maximum ozone measurement that is above the level of the standard. Therefore the phrase "expected number of exceedances" is equivalent to "the expected number of daily maximum ozone values above the level of the standard."

1.3. Basic Premises

By its very nature, the existence of a guideline document implies several things: (1) that there is a problem, (2) that a solution is provided, and (3) that there were several alternatives considered in reaching the solution. Obviously, if there is no problem then the guideline is of limited value, and if there were not some alternative solutions then the guidance is perhaps superfluous or at best educational. The third point indicates that the "best" alternative, in some sense, was selected. With this in mind, it is useful to briefly discuss some of the key points that were considered in judging the various options. The purpose of this section is to briefly indicate the criteria used in developing this particular guideline.

The most obvious criterion is simplicity. This simplicity extends to several aspects of the problem. When someone asks if a particular area meets the standard they expect either a "yes" or "no" as the answer or even an occassional "I don't know". Secondly, this simplicity should extend to the reason why the standard was met or violated. If a panel of experts is required to debate the probability that an area is in compliance then the general public may rightly feel confused about just what is being done to protect their health. Also,

the more clear-cut the status of an area is (and the reasons why) the more likely it is that all groups involved can concentrate on the real problem of maintaining clean air rather than arguing over minor side issues.

While simplicity is desirable, if the problem is complex the solution cannot be oversimplified. In other words, the goal is to develop a solution that is simple, and yet not simple-minded. In order to do this, the approach taken in this document is to recognize that there are two questions involved in determining compliance: (1) was the standard violated? and (2) if so, by how much? The first question is the simpler of the two in that a "yes/no" answer is expected. The second question implies both a quantification and a determination of what to do about it. Therefore, it seems reasonable to have a more complicated procedure for determining the second answer.

In addition to the trade-offs between simplicity and complexity another problem is to allow a certain amount of flexibility without being vague. There are several reasons for allowing some degree of flexibility. Not only do available resources vary from one area to another but the complexity of the air pollution problems vary. An area with no pollution problem should not be required to do an extensive analysis just because that level of detail is needed someplace else. Conversely, an area with sufficient resources to perform a detailed analysis of their pollution problem to develop an optimum control strategy should not be constrained from doing so simply because it is not warranted elsewhere. Furthermore, a certain degree of flexibility is essential to allow for modified monitoring schedules that are used to make the best use of available resources.

In addition to these points concerning simplicity and flexibility, certain other considerations are of course involved. In particular, the methodology employed cannot merely ignore high values for a particular year simply because they are unlikely to reoccur. The purpose of the standard is to protect against high values in a manner consistent with the likelihood of their occurrence.

A final point is that the proposed interpretation

should involve a framework that could eventually be extended to other pollutants, if necessary, and easily modified in the future as our knowledge and understanding of air pollution increases.

It should be noted that no specific mention is made of measurement error in the following discussions. While it would be naive to assume that measurement errors do not occur, at the present time it is difficult to allow for measurement errors in a manner that is not tantamount to re-defining the level of the standard. Obviously there is no question that data values known to be grossly in error should be corrected or eliminated. In fact the use of multiple years of data for the ozone standards should facilitate this process. The more serious practical problem is with the level of uncertainty associated with every individual measurement. The viewpoint taken here is that these inherent accuracy limitations are accounted for in the choice of the level of the standard and that equitable risk from one area to another is assured by use of the reference (or an equivalent) ambient monitoring method and adherence to a required minimum quality assurance program. It should be noted that the stated level of the standard is taken as defining the number of significant figures to be used in comparisons with the standard. For example, a standard level of .12 ppm means that measurements are to be rounded to two decimal places (.005 rounds up), and, therefore, .125 ppm is the smallest concentration value in excess of the level of the standard.

2. ASSESSING COMPLIANCE

This section examines the ozone standard with particular attention given to the evaluation of compliance. This is done in several steps. The first is a discussion of the term "expected number." Once this is defined it is possible to consider the interpretation when applied to several years of data or to less than complete sampling data. An example calculation is included at the end of this section to summarize and illustrate the major points.

2.1. Interpretation of "Expected Number"

The wording of the ozone standard states that the "expected number of days per calendar year" must be "equal to or less than 1." The statistical term "expected number" is basically an arithmetic average. Perhaps the simplest way to explain the intent of this wording is to give an example of what it would mean for an area to be in compliance with this type of standard. Suppose an area has relatively constant emissions year after year and its monitoring station records an ozone value for every day of the year. At the end of each year the number of daily values above the level of the standard is determined and this is averaged with the results of previous years. As long as this arithmetic average remains "less than or equal to 1" the area is in compliance. As far as rounding conventions are concerned, it suffices to carry one decimal place when computing the average. For example, the average of the three numbers 1,1,2 is 1.3 which is greater than 1.

Two features in this example warrant additional discussion to clearly define how this proposal would be implemented. The example assumes that a daily ozone measurement is available for each day of the year so that the number of exceedances for the year is known. On a practical basis this is highly unlikely and, therefore, it will be necessary to estimate this quantity. This is discussed in section 2.2. In the example it is also assumed that several years of data are available and there is relatively little change in

emissions. This is discussed in more detail in section 2.3.

The key point in the example is that as data from additional years are incorporated into the average this expected number of exceedances per year should stabilize. If unusual meteorology contributes to a high number of exceedances for a particular year then this will be averaged out by the values for other "normal" years. It should be noted that these high values would, therefore, not be ignored but rather their relative contribution to the overall average is in proportion to the likelihood of their occurrence. This use of the average may be contrasted with an approach based upon the median. If the median were used then the year with the greatest number of exceedances could be ignored and there would be no guarantee of protection against their periodic reoccurrence.

2.2. Estimating Exceedances for a Year

As discussed above, it is highly unlikely that an ozone measurement will be available for each day of the year. Therefore, it will be necessary to estimate the number of exceedances in a year. The formula to be used for this estimation is contained in Appendix H of the ozone standard. The purpose of this section is to present the same basic formula but to expand upon the rationale for choosing this approach and to provide illustrations of certain points.

Throughout this discussion the term "missing value" is used in the general sense to describe all days that do not have an associated ozone measurement. It is recognized that in certain cases a so-called "missing value" occurs because the sampling schedule did not require a measurement for that particular day. Such missing values, which can be viewed as "scheduled missing values," may be the result of planned instrument maintenance or, for ozone, may be a consequence of a seasonal monitoring program. In order to estimate the number of exceedances in a particular year it is necessary to account for the possible effect of missing values. Obviously, allowance for missing values can only result in an estimated number of exceedances at least as large as the observed number. From a practi-

cal viewpoint, this means that any site that is in violation of the standard based upon the observed number of exceedances will not change status after this adjustment. Thus, in a sense, this adjustment for missing values is required to demonstrate attainment, but may not be necessary to establish non-attainment.

In estimating the number of exceedances in cases with missing data, certain practical considerations are appropriate. In some areas, cold weather during the winter makes it very unlikely that high ozone values would occur. Therefore it is possible to discontinue ozone monitoring in some localities for limited time periods with little risk of incorrectly assessing the status of the area. As indicated in Appendix H, the proposed monitoring regulations(CFR58) would permit the appropriate Regional Administrator to waive any ozone monitoring requirements during certain times of the year. Although data for such a time period would be technically missing, the estimation formula is structured in terms of the required number of monitoring days and therefore these missing days would not affect the computations.

Another point is that even though a daily ozone value is missing, other data might indicate whether or not the missing value would have been likely to exceed the standard level. There are numerous ways additional information such as solar radiation, temperature, or other pollutants could be used but the final result should be relatively easy to implement and not create an additional burden. An analysis of 258 site-years of ozone/oxidant data from the highest sites in the 90 largest Air Quality Control Regions showed that only 1% of the time did the high value for a day exceed .12 ppm if the adjacent daily values were less than .09 ppm. With this in mind the following exclusion criterion may be used for ozone:

A missing daily ozone value may be assumed to be less than the level of the standard if the daily maxima on both the preceding day and the following day do not exceed 75% of the level of the standard.

It should be noted that to invoke this exclusion criterion data must be available from both adjacent days. Thus it does not apply to consecutive missing

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daily values. Having defined the set of missing values that may be assumed to be less than the standard it is possible to present the computations required to adjust for missing data.

Let z denote the number of missing values that may be assumed to be less than the standard. Then the following formula shall be used to estimate the number of exceedances for the year:

$$e=v+(v/n)*(N-n-z) \qquad (1)$$

(* indicates multiplication)

Where N = the number of required monitoring days in the year

n = the number of valid daily maxima

v = the number of measured daily values above the level of the standard

z = the number of days assumed to be less than the standard level, and

e = the estimated number of exceedances for the year.

This estimated number of exceedances shall be rounded to one decimal place (fractional parts equal to .05 round up).

Note that N is always equal to the number of days in the year unless a monitoring waiver has been granted by the appropriate Regional Administrator.

The above equation may be interpreted intuitively in the following manner. The estimated number of exceedances is equal to the observed number plus an increment that accounts for incomplete sampling. There were (N-n) missing daily values for the year, but a certain number of these, namely z, were assumed to be below the standard. Therefore, (N-n-z) missing values are considered to be potential exceedances. The fraction of measured values that were above the level of

the standard was v/n and it is assumed that the same fraction of these candidate missing values would also exceed the level of the standard.

The estimation procedures presented are computationally simple. Some data processing complications result when missing data are screened to ensure a representative data base, but on a practical basis this effort is only required for sites that are marginal with respect to compliance. Because the exclusion criterion for missing values does not differentiate between scheduled and non-scheduled missing values it is possible to develop a computerized system to perform the necessary calculations without requiring additional information on why each particular value was missing. In principle, if allowance is made for missing values that are relatively certain to be less than the standard then it would seem reasonable to also account for missing values that are relatively certain to be above the standard. Although this is a possibility, it will probably not be necessary initially because such a situation would, of necessity, have at least two values greater than the standard level. Therefore, it is quite likely that this would be an unnecessary complication in that it would not affect the assessment of compliance.

One feature of these estimation procedures should be noted. If an area does not record any values above the standard, then the estimated number of exceedances for the year is zero. An obvious consequence of this is that any area that does not record a value above the standard level will be in compliance. In most cases this confidence is warranted. However, at least some qualification is necessary to indicate that it is possible that the existing monitoring data can be deemed inadequate for use with these estimation formulas. In general, data sets that are 75% complete for the peak pollution potential seasons will be deemed adequate. Although the general 75% completeness rule has been traditionally used as an air quality validity criterion the key point is to ensure reasonably complete monitoring of those time periods with high pollution potential. An additional word of caution is probably required at this point concerning attainment status determinations based upon limited data. If a particular area has very limited data and shows no exceedances of the standard it must be recognized that a more intense

monitoring program could possibly result in a determination of non-attainment. Therefore, if it is critical to immediately determine the status of a particular area and the ambient data base is not very complete, the design value computations presented in section 3 may be employed as a guide to assess potential problems. The point is, that as the monitoring data base increases, the additional data may indicate non-attainment. Therefore some caution should be used when viewing attainment status designations based upon incomplete data.

2.3. Extension to Multiple Years

As discussed earlier, the major change in the ozone standard is the use of the term "expected number" rather than just "the number." The rationale for this modification is to allow events to be weighted by the probability of their occurrence. Up to this point, only the estimation of the number of exceedances for a single year has been discussed. This section discusses the extension to multiple years.

Ideally, the expected number of exceedances for a site would be compared by knowing the probability that the site would record 0,1,2,3,... exceedances in a year. Then each possible outcome could be weighted according to its likelihood of occurrence, and the appropriate expected value or average could be computed. In practice, this type of situation will not exist because ambient data will only be available for a limited number of years.

A period of three successive years is recommended as the basis for determining attainment for two reasons. First, increasing the number of years increases the stabiity of the resulting average number of exceedances. Stated differently, as more years are used, there is a greater chance of minimizing the effects of an extreme year caused by unusual weather conditions. The second factor is that extending the number of successive years too far increases the risk of averaging data during a period in which a real shift in emissions and air quality has occurred. This would penalize areas showing recent improvement and similarly reward areas which are experiencing deteriorating ozone

air quality. Three years is thought by EPA to represent a proper balance between these two considerations. This specification of a three year time period for compliance assessment also provides a firm basis for purposes of decision-making. While additional flexibility is possible for developing design values for control strategy purposes, a more definitive framework seems essential when judging compliance to eliminate possible ambiguity and to clearly identify the basis for the decision.

Consequently, the expected number of exceedances per year at a site should be computed by averaging the estimated number of exceedances for each year of data during the past three calendar years. In other words, if the estimated number of exceedances has been computed for 1974, 1975, and 1976, then the expected number of exceedances is estimated by averaging those three numbers. If this estimate is greater than 1, then the standard has been exceeded at this site. As previously mentioned, it suffices to carry one decimal place when computing this average. This averaging rule requires the use of all ozone data collected at that site during the past three calendar years. If no data are available for a particular year then the average is computed on the basis of the remaining years. If in the previous example no data were available for 1974, then the average of the estimated number of exceedances for 1975 and 1976 would be used. In other words, the general rule is to use data from the most recent three years if available, but a single season of monitoring data may still suffice to establish non-attainment. Thus, this three year criterion does not mean that non-attainment decisions must be delayed until three years of data are available. It should be noted that to establish attainment by a particular date, allowance will be permitted for emission reductions that are known to have occurred.

One point worth commenting on is the possibility that the very first year is "unusual." While this could occur, in the case of ozone most urbanized areas already have existing data bases so that some measure of the normal number of exceedances per year is available. Furthermore the nature of the ozone problem makes it unlikely that areas currently well above the standard would suddenly come into compliance. Therefore, as these areas approach the standard addi-

tional years of data would be available to determine the expected number of exceedances for a year.

2.4. Example Calculation

In order to illustrate the key points that have been discussed in this section it is convenient to consider the following example for ozone.

Suppose a site has the following data history for 1978-1980:

1978: 365 daily values; 3 days above the standard level.

1979: 285 daily values; 2 days above the standard level; 21 missing days satisfying the exclusion criterion.

1980: 287 daily values; 1 day above the standard level; 7 missing days satisfying the exclusion criterion.

Suppose further that in 1980 measurements were not taken during the months of January and February (a total of 60 days for a leap year) because the cold weather minimizes any chance of recording exceedances and a monitoring waiver had been granted by the appropriate Regional Administrator.

Because the three year average number of exceedances is clearly greater than 1, there is no computation required to determine that this site is not in compliance. However, the expected number of exceedances may still be computed using equation 1 for purposes of illustration.

For 1978, there were no missing daily values and

therefore there is no need to use the estimated exceedances formula. The number of exceedances for 1978 is 3.

For 1979, equation 1 applies and the estimated number of exceedances is:

$$2 + (2/285)*(365 - 285 - 21) =$$

$$2 + 0.4 = 2.4$$

For 1980, the same estimation formula is used but due to the monitoring waiver for January and February the number of required monitoring days is 306 and therefore the estimated number of exceedances is:

$$1 + (1/287)*(306 - 287 - 7) =$$
$$1 + (1/287)*(12) = 1.0$$

Averaging these three numbers (3, 2.4, and 1.0) gives 2.1 as the estimated expected number of exceedances per year and completes the required calculations.

3. ESTIMATING DESIGN VALUES

The previous section addressed compliance with the standard. As discussed, it suffices to treat questions concerning compliance as requiring a "yes/no" type answer. This approach facilitates the use of relatively simple computational formulas. It also makes it unnecessary to define the type of statistical distribution that describes the behavior of air quality data. The advantage of not invoking a particular statistical distribution is that the key issue of whether or not the standard is exceeded is not obscured by which particular distribution best describes the data. However, once it is established that an area exceeds the standard, the next logical question is more quantitative and requires an estimate of by how much the standard was exceeded. This is done by first examining the definition of a design value for an "expected exceedances" standard and then discussing various procedures that may be used to estimate a design value. A variety of approaches are considered such as fitting a statistical distribution, the use of conditional probabilities, graphical estimation, and even a table look-up procedure. In a sense each of these approaches should be viewed as a means to an end, i.e., meeting the applicable air quality standard. As long as this final goal is kept in mind any of these approaches are satisfactory. As with the previous section discussing compliance, this section concludes with example calculations illustrating the more important points.

3.1. Discussion of Design Values

In order to determine the amount by which the standard is exceeded it is necessary to discuss the interpretation of a design value for the proposed standard. Conceptually the design value for a particular site is the value that should be reduced to the standard level thereby ensuring that the site will meet the standard. With the wording of the ozone standard the appropriate design value is the concentration with expected number of exceedances equal to 1. Although this describes the design value in words it is useful

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to introduce certain notations to precisely define this quantity.

Let $P(x \leq c)$ denote the probability that an observation x is less than or equal to concentration c. This is also denoted as F(c).

Let e denote the number of exceedances of the standard level in the year, e.g., in the case of ozone this would be the number of daily values above .12 ppm. Then the expected value of e denoted as E(e) may be written as:

$$E(e) = P(x > .12) * 365 = [1 - F(.12)] * 365$$

For a site to be in compliance the expected number of exceedances per year E(e), must be less than or equal to 1. From the above equation it follows that this is equivalent to saying that the probability of an exceedance must be less than or equal to 1/365.

As indicated, the appropriate design value is that concentration which is expected to be exceeded once per year. Alternatively, the design value is chosen so that the probability of exceeding this concentration is 1/365. If an equation is known for F(c) then the design value may be obtained by setting 1-F(c) equal to 1/365 and solving for c. If a graph of F(c) is known then the design value may be determined graphically by choosing the concentration value that corresponds to a frequency of exceedance of 1/365. Obviously in practice the distribution F(c) is not really known. What is known is a set of air quality measurements that may be approximated by a statistical distribution to determine a design value as discussed in the following section.

3.2. The Use of Statistical Distributions

The use of a statistical distribution to approximately describe the behavior of air quality data is certainly not new. The initial work by Larsen [4] with the log-normal distribution demonstrated how this type

of statistical approximation could be used. The proposed form of the ozone standard provides a framework for the use of statistical distributions to assess the probability that the standard will be met. An important point in dealing with air pollution problems is that the main area of interest is the high values. The National Ambient Air Quality Standards are intended to limit exposure to high concentrations. This has a direct impact on how statistical distributions are chosen to describe the data. [5] If the intended application is to approximate the data in the upper concentration ranges then obviously it must be required that any statistical distribution selected for this purpose has to fit the data in these higher concentration ranges. Initially this would appear to be an obvious truism but, in many cases, a particular distribution may "reasonably approximate" the data in the sense that it fits fairly well for the middle 80% of the values. This may be satisfactory for some applications but if the top 10% of the data is the range of interest it may be inappropriate.

Over the years various statistical distributions have been suggested for possible use in describing air quality data. Example applications include the two-parameter lognormal[4], the three-parameter lognormal[6], the Weibull[5,7], and the exponential distribution[5,8]. Despite certain theoretical reservations concerning factors such as interdependence of successive values these approaches have been proven over time to be useful tools in air quality data analysis. The appropriate choice of a distribution is useful in determining the design value. Viewed in perspective, however, the selection of the appropriate statistical distribution is a secondary objective -- the primary objective is to determine the appropriate design value. In other words, the question of interest is "what concentration has an expected number of exceedances per year equal to 1?" and not "which distribution perfectly describes the data?" Therefore, it is not necessary to require that any particular distribution be used. All that is necessary is to indicate the characteristics that must be considered in determining what is meant by a "reasonable fit". In fact it will be seen later that a design value may be selected without even knowing which particular distribution best describes the data.

There are certain points that are implicit in the above discussion which are worth commenting upon. One possible approach in developing this type of guidance is to specify a particular distribution to be used in determining a design value. This approach is not taken here for a variety of reasons. There is no guarantee that one family of distributions would be adequate to describe ozone levels for all areas of the country, for all weather conditions, etc. It may well be that different distributions are needed for different areas. Secondly, as control programs take effect and pollution levels are reduced the so-called "best" distribution may change. Another point that should be emphasized involves the distinction between determining compliance and determining a design value. Suppose, for example, that a statistical distribution is selected and adequately describes all but the highest five values each year. However, these five values are always above the standard and consequently the number of exceedances per year is always five. Such a site is not in compliance even if the design value predicted from the approximating distribution is below the standard level. In such a case the expected number of exceedances per year is 5 (with complete sampling) and therefore the site is in violation. The design value is an aid in determining the general reduction required, but it some cases it may be necessary to further refine the estimate because of inadequate fit for the high values.

3.3. Methodologies

The purpose of this section is to present some acceptable approaches to determine an appropriate design value, i.e., the concentration with expected number of exceedances per year equal to 1. As discussed, this may be alternatively viewed as determining the concentration that will be exceeded 1 time out of 365.

Throughout this discussion it is important to recognize that the number of measurements must be treated properly. In particular, missing values that are known to be less than the standard level should be accounted for so that they do not incorrectly affect the empirical frequency distribution. For example, if an area does not monitor ozone in December, January, and February, because no values even approaching the stan-

dard level have ever been reported in these months then these observations should not be considered missing but should be assigned some value less than the standard. The exact choice of the value is arbitary and is not really important because the primary purpose is to fit the upper tail of the distribution.

In discussing the various acceptable approaches several different cases are presented. This is intended to illustrate the general principles that should be applied in determining the design value. Throughout these discussions it is generally assumed that more than one year of data is available. The difficulty with using a single year of data is that any effect due to year to year variations in meteorology is obviously not accounted for. Therefore, any results based upon only one year of data should be viewed as a guide that may be subject to revision.

(1) Fitting One Statistical Distribution to Several Years of Data

One of the simplest cases is when several years of fairly complete data are available during a time of relatively constant emissions. In this situation the data can be plotted to determine an empirical frequency distribution. For example, all data for a site from a 3-5 year period could be ranked from smallest to largest and the empirical frequency distribution plotted on semi-log paper. This type of plot emphasizes the behavior of the upper tail of the data as shown in Figure 1. A discussion of this plotting is contained elsewhere. [5] Figure 2 illustrates how different types of distributions would appear on such a plot. The data may also be plotted on other types of graph paper, such as log-normal or Weibull. The ideal situation is when the data points lie approximately on a straight line. The next step is to choose a statistical distribution that approximately describes the data and to fit the distribution to the data. This may be done by least squares, maximum likelihood estimation, or any method that gives a reasonable fit to the top 10% of the data. An obvious question is "what constitutes a reasonable fit?" This can be judged visually by plotting the fitted distribution on the same graph as the data points. Because of the intended use of the distribution the degree of approximation for the top

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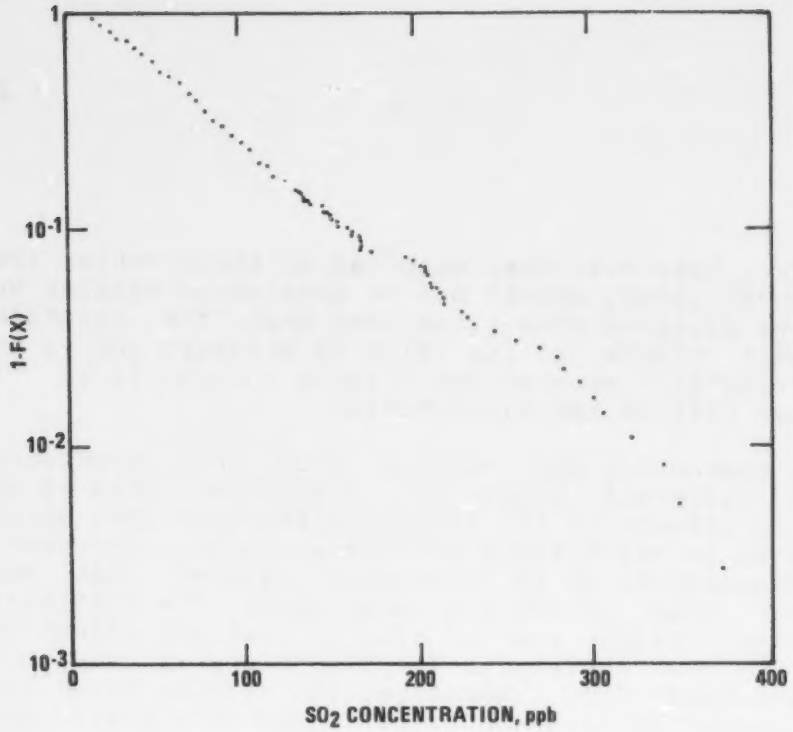

Figure 1. Sulfur dioxide measurements for 1968 (24-hour) at CAMP station in Philadelphia, Pa., plotted on semi-log paper.

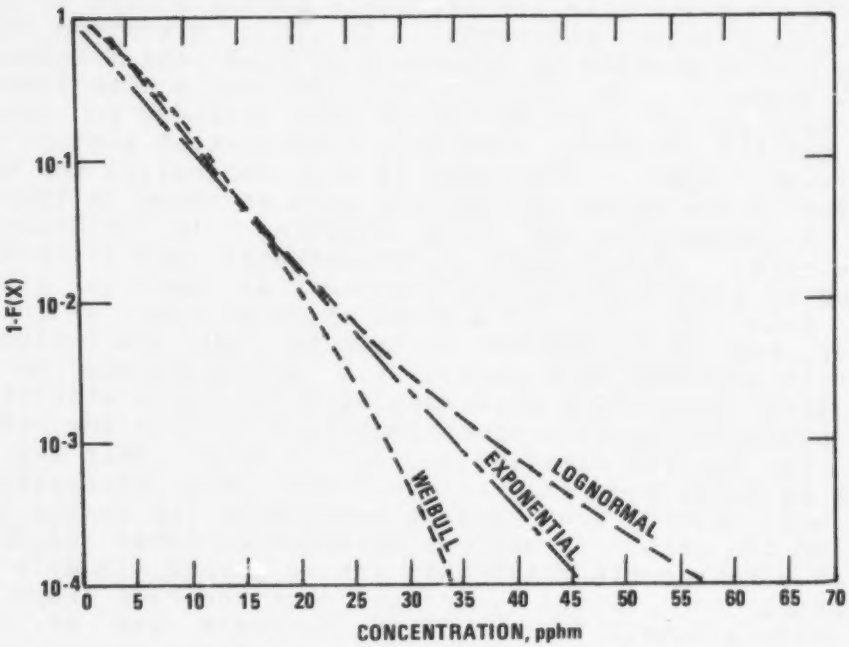

Figure 2. Examples of lognormal, exponential, and Weibull distributions plotted on semi-log paper. A Weibull distribution may also curve upward for certain parameter values.

10%, 5%, 1% and even .5% of the data must be examined. The most obvious check is to examine departures of the actual data points from the fitted distribution. As a general rule there should be no obvious pattern to the lack of fit in terms of under- or over-prediction ,or trend. For example, if the fitted distribution underestimates all of the last eight data points by more than 5%, then it must be established that the fitted distribution is reasonable. Such an argument might involve showing that the majority of these data points all occurred in the same period and that the meteorology for these particular days was extremely unusual. The claim that this meteorology was unusual would also have to be substantiated by examining historical meteorological data. It should be noted that this extra effort is not routinely required and would only be necessary when the fit appears inadequate. The design value corresponds to a frequency of 1/365 and in some cases the empirical frequency distribution function will be plotted in this range. In such cases, the fitted distribution should be consistent with the empirical distribution in this range. This can be examined graphically by locating the concentration on the empirical frequency distribution function corresponding to a frequency of 1/365. By construction, there will be measured data points on either side of this value. The two measured concentrations below this value and the two measured concentrations above this value will be used as a constraint in fitting a distribution. If the fitted distribution results in a design value that differs by more than 5% from all four of these measured concentrations, some explanation should be presented indicating the reasons for this discrepancy. It should be noted that in some cases there may be only one, rather than two, measured values on the empirical frequency distribution with frequencies less than 1/365. In these cases the upper constraint would consist of one rather than two data points.

(2) Using the Empirical Frequency Distribution of Several Years of Data (Graphical Estimation)

It should be noted that if several years of fairly complete data are available it is not necessary to even fit a statistical distribution. The concentration value corresponding to a frequency of 1/365 may be read directly off the graph of the empirical distribution

Table 1.

TABULAR ESTIMATION OF DESIGN VALUE

Number of Daily Values	Rank of Upper Bound	Rank of Lower Bound	Data Point Used for Design Value
365 to 729	1	2	highest value
730 to 1094	2	3	second highest
1095 to 1459	3	4	third highest
1460 to 1824	4	5	fourth highest
1825 to 2189	5	6	fifth highest

function and used as the design value.

If the data records are not sufficiently complete then the empirical distribution function will not be plotted for the 1/365 frequency and it will be necessary to fit a distribution to estimate the design value. However, whenever sufficient data are available, this technique provides a convenient means of graphically estimating the design value.

(3) Table Look-up

An obvious point that can initially be overlooked in the discussion of these techniques is that the final choice of a design value is primarily influenced by the few highest values in the data set. With this in mind, it is possible to construct a simple table look-up procedure to determine a design value. Again, it is important to treat the number of values properly to ensure that the data adequately reflects all portions of the year.

To use this tabular approach it is only necessary to know the total number of daily values, and then determine a few of the highest data values,. For example, if there are 1,017 daily values then the ranks of the lower and upper bounds obtained from Table 1 are 3 and 2. This means that an appropriate design value would be between the third- highest and second-highest observed values. In using this table the higher of the two concentrations may be used as the design value. Therefore in this particular case, it suffices to know the three highest measured values during the time period.

This look-up procedure is basically a tabular technique for determining what point on the empirical frequency distribution corresponds to a frequency of 1/365. By construction, the table look-up procedure overestimates the design value. For instance, in the example with 1,017 values an acceptable design value would lie closer to the lower bound. This could be handled by interpolation between the second and third highest values. However, rather than introduce interpolation formulas it would be simpler to merely use the previously discussed graphical procedure.

For the cases that are 75% complete but still have less than 365 days the maximum observed concentration may be used as a tentative design value as long as the data set was 75% complete during the peak times of the year. In this case it must be recognized that the design value is quite likely to require future revision. In principle, if statistical independence applied, this maximum observed concentration would equal or exceed the 1/365 concentration about half the time. However, the failure to adequately account for yearly variations in meteorology makes any estimate based on a single year of data very tentative.

(4) Fitting a Separate Distribution for Each Year of Data (Conditional Probability Approach)

The previous method required grouping data from several years into a single frequency distribution. In some cases data processing constraints may make this cumbersome. Therefore, an alternate approach may be used that allows each year to be treated individually. In considering this alternate approach it is useful to briefly indicate the underlying framework. This particular approach uses conditional probabilities and in most cases it would probably be more convenient to use one of the previous methods. However, the underlying framework of this method has sufficient flexibility to warrant its inclusion.

Suppose that the air quality data at a particular site may be approximated by some statistical distribution $F(x|\theta)$, where θ denotes the fitted parameters. Suppose further that the values of the fitted parameters differ from year to year, but that the data may still be approximated by the same type of distribution. Intuitively this would mean that while the same type of distribution describes each year of data, the values of the parameters would change from year to year reflecting the prevailing meteorology for the year. In theory it could be possible to define a set of meteorological classes, say $m(i)$, so that the distribution function of the air quality data could be defined for each one of these meteorological classes. Then for each meteorological class, $m(i)$, there would be an associated air quality distribution function denoted as $F(x|m(i))$, the distribution function for x given the meteorological class $m(i)$. Using the standard rules of

conditional probability the distribution function F(x) may be written as:

$$F(x) = \sum_i \{F(x|m(i))\}\, P[m(i)]$$

where P[m(i)] is the probability of meteorological class m(i) occurring.

Continuing this approach the expected number of exceedances may be written as:

$$E(e) = \sum_i P[x > s\,|m(i)] * P[m(i)]$$

where s denotes the standard level.

Initially the above framework may seem to be too theoretical to have much practical use. However, it will be seen in Section 4 that this approach may afford a convenient means of determining the expected number of exceedances per year when limited historical data is available. For the present discussion it suffices to indicate how this approach may be used when ambient data sets are available.

Suppose that five years of ambient measurements are available. An approximating statistical distribution may be determined as discussed previously for each year, denoted as Fi(x). This would be analogous to the F(x|m(i)) in the above discussion. Then the distribution function of F(x) may be written as:

$$F(x) = \sum_{i=1}^{5} Fi(x) * 1/5$$

where Fi is analogous to F[x|m(i)] and P[m(i)] is assumed to be 1/5. The design value may then be determined by setting 1-F(d) = 1/365 and solving for d, the design value. This is equivalent to determining the concentration d so that:

$$\sum_{i=1}^{5} [1-Fi(d)] * 1/5 = 1/365.$$

In general it may not be possible to explicity solve this equation for d, but the answer may be obtained iteratively by first guessing an appropriate design value.

The use of this equation can perhaps best be illustrated by a simple example with two years of data. Suppose the data for each year may be approximated by an exponential distribution although the parameter is different for the two years. In particular let

$$F1(x) = 1 - EXP(-43.4x) \quad \text{and}$$
$$F2(x) = 1 - EXP(-37.6x).$$

Using the previous equation, the design value (d) must be determined so that

$$1/2\ EXP(-43.4d) + 1/2\ EXP(-37.6d) = 1/365 \quad \text{or}$$
$$365 * \{1/2\ EXP(-43.4d) + 1/2\ EXP(-37.6d)\} = 1.$$

If .15 is used as an initial guess for d this equation gives a value of .92 rather than 1. If .145 is used the resulting value is 1.12 indicating that the design value is between .145 and .15. Guessing .148 gives a value of .99,i.e.

$$365\{1/2\ EXP(-43.4 * .148) + 1/2\ EXP(-37.6 * .148)\} = .99$$

This is sufficiently close to 1 and is a reasonable stopping place in determining the design value.

3.4. Quick Test for Design Values

All of the approaches in the previous section have one thing in common; namely, their purpose. Each technique is intended to select an appropriate design value, i.e., a concentration with expected number of

yearly exceedances equal to 1. With this in mind a quick check may be made to determine how reasonable the selected design value is. This may be done by counting the number of observed daily values that exceed the selected design value and computing the average number of exceedances per year. For example, if the selected design value was exceeded 4 times in 3 years, then the average number of exceedances per year is 1.3. Ideally, this average should be less than or equal to 1, but for a variety of reasons somewhat higher values may occur. However, if this average is greater than 2.0 the design value is questionable. In such cases the design value should either be changed or, if not changed, careful examination should be performed to substantiate this choice of a design value.

3.5. Discussion of Data Requirements

The use of the previous approaches presupposes the existence of an adequate data base. Both approaches were presented in the context of having several years of ambient data. In many practical cases the available data base may not be so extensive. Although these statistical approaches may be used with less data, some caution is still required to ensure a minimally acceptable data set. In general, statistical procedures permit inferences to be made from limited data sets. Nevertheless, the initial data set must be representative. For example, if no data is available from the peak season, then any extrapolations would require more than merely statistical procedures. Therefore, the input data sets should be at least 50% complete for the peak season with no systematic pattern of missing potential peak hours. This 50% completeness criterion should be viewed in the context of the type of monitoring performed. A continuous monitor that fails to produce data sets meeting this criteria has in effect a down-time of more than 50%. With such a high percentage of down-time for the instrument even the recorded values should be viewed with caution.

In employing approaches that group data from all years into one frequency distribution, it should be verified that all years have approximately the same pattern of missing values. Furthermore, if the number of measurements during the oxidant season differs by

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more than 20% from one year to another, then the conditional probability approach should be used. The reason for this constraint is to ensure that variations in sample sizes do not result in disproportionate weighting of data from different years.

Another point of concern is how many years of data should be used. Intuitively it would be reasonable to use as many years of data as possible as long as emissions have not changed "appreciably". Obviously this suggests that some guidance be provided on what percent change in emissions is permissible. To some degree any such specification is arbitrary. However, the more relevant point is that the specified percentage be reasonable. The reason for a cut-off is to ensure that the impact of increased emissions is not masked by the use of air quality data occurring prior to these emission increases. If an area is in violation of the standard, then emission changes should be expected as control programs take effect. Also, the design value serves as a guide to achieving the standard and is, in a sense, merely the means to an end rather than an end in itself. Therefore, no more than a 20% variation between the lowest and highest years is recommended. It should be noted that a total variation of 20% may translate into a + or - 10% variation around the average.

If emissions have increased by more than 20% then additional years should not be incorporated unless the air quality values can be adjusted for the change in emissions. For cases in which emissions have decreased by more than 20% the earlier data may be used after adjustment or used without change knowing that the design value will consequently be conservative. Although this document does not discuss methods for performing this adjustment, it is useful to mention the basic principle involved. The selection of a design value inherently implies the existence of an acceptable model for taking an air quality value and determining the emission reduction required to reduce this value to the standard. In principle, then, this same model may be used in reverse to take the emission change known to have occurred and use the model to scale the previous data sets. Attempting to adjust older historical data may initially seem to be an unnecessary complication but the more data that can be used to estimate the design value the more likely it is that a proper design

value is selected. Because considerable effort could be expended in revising a control strategy this additional effort may be warranted.

3.6. Example Design Value Computations

As in the previous discussion of compliance assessment, it is convenient to conclude this section with examples illustrating the main point involved in applying these various techniques. For purposes of illustration all four techniques are used on the same data set. Figures 3,4, and 5 display semi-log plots of daily ozone values for 1974, 1975 and 1976 at a sample site. These data are plotted using previously discussed conventions. [5] The horizontal axis is concentration (in ppm) and the vertical axis is the fraction of values exceeding this concentration. A horizontal dotted line is shown at a frequency of 1/365 and the dotted line represents a Weibull distribution approximating the data. This particular fit was done by "eye-balling" the data, but suffices for the purposes of illustration. Figure 6 is a similar plot for all three years of data grouped together. The high and second high values for the three years are: (.13 and .12), (.16 and .16), and (.15 and .14).

Method 1: Fitting a single distribution to data from all three years.

The Weibull distribution plotted in Figure 6 for the three years of data is described by the equation:

$$F(x) = 1 - \mathrm{EXP}[-(x/.0609)^{2.011}].$$

Setting $F(x) = 1 - 1/365$ and solving for x gives .147 which is the design value because it corresponds to a frequency of exceedance of 1/365. Using this quick check, there are three values above .147 so the average number of yearly exceedances is 1.

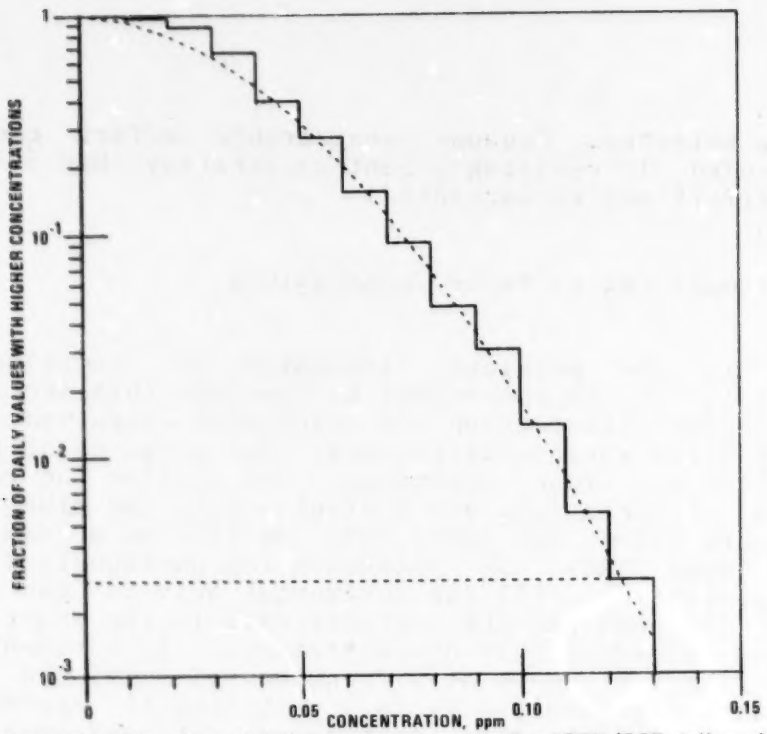

Figure 3. Semi-log plot of daily maximum ozone for 1975 (365 daily values).

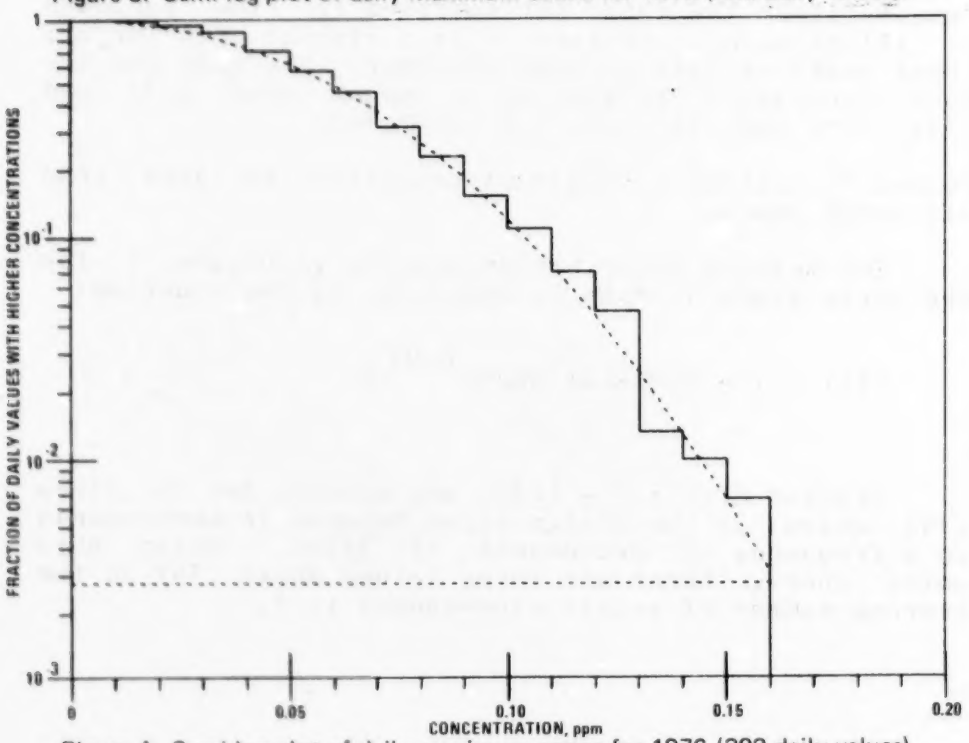

Figure 4. Semi-log plot of daily maximum ozone for 1976 (303 daily values).

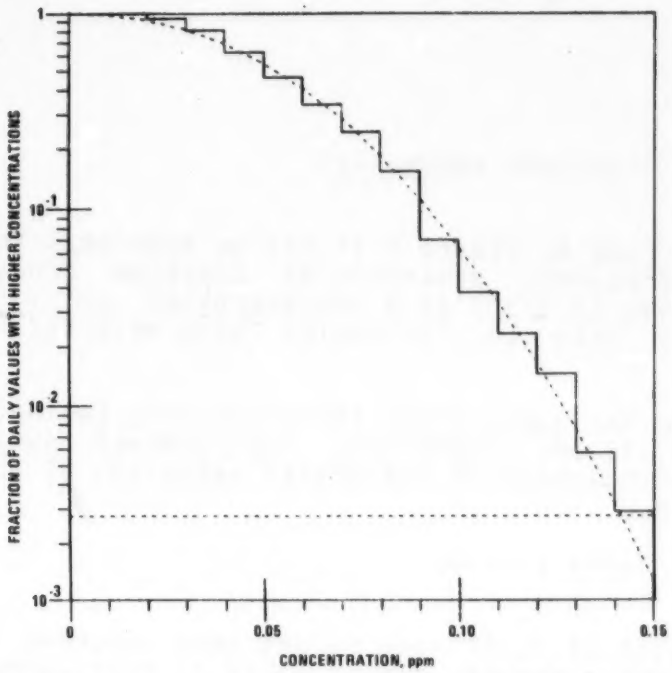

Figure 5. Semi-log plot of daily maximum ozone for 1977 (349 daily values).

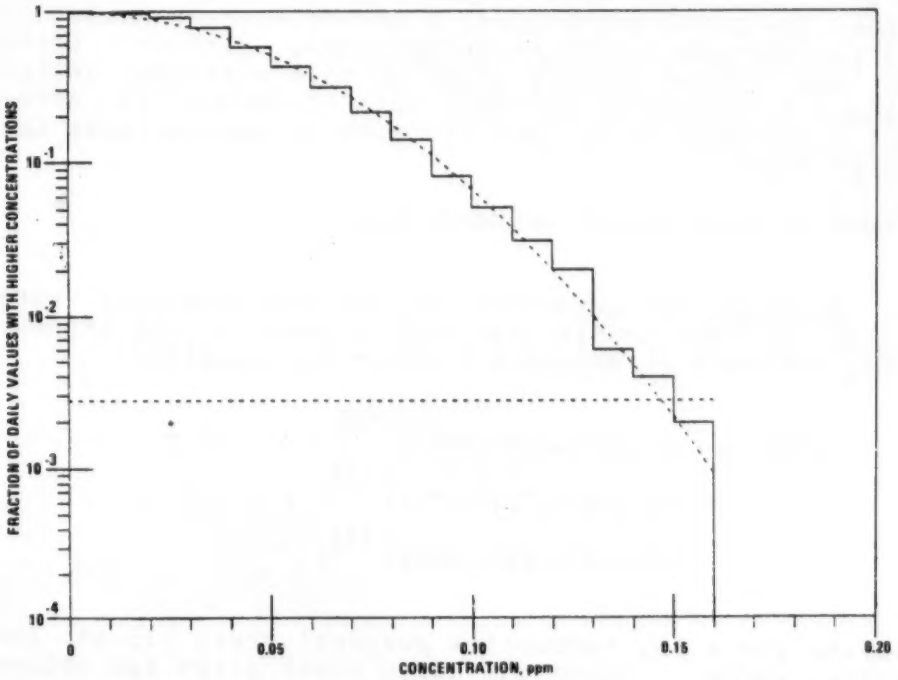

Figure 6. Semi-log plot of daily maximum ozone for three years: 1975, 1976, 1977 (1,017 daily values).

Method 2: Graphical estimation

Referring to Figure 6 it may be seen that the empirical frequency distribution function crosses the line plotted at 1/365 at a concentration of .15 and, therefore, this is the design value selected by this method.

Using the quick check there are only two data values above .15 and, therefore, the average number of yearly exceedances of the design value is .67 which is acceptable.

Method 3: Table look-up

A total of 1,017 data values were recorded during the three year period. Using Table 1, this method says that the second highest value may be used as the design value. Therefore this method yields .16 as the design value. The quick check gives 0 as the average number of yearly exceedances of the design value although there are two values exactly equal to this estimated design value. As indicated earlier, this procedure is somewhat conservative in that it tends to overestimate the design value.

Method 4: Conditional probabilities

Separate two parameter Weibull distributions were fitted to each yearly data set as shown in the graphs. Using the form of equation 5 gives the equation:

$$1/365 = 1/3\ \mathrm{EXP}\{-(d/.0467)^{1.835}\} + 1/3\ \mathrm{EXP}\{-(d/.0705)^{2.139}\} + 1/3\ \mathrm{EXP}\{-(d/.0629)^{2.180}\}$$

Solving for d (by successive guesses) gives .15 as the design value. Using the quick check gives two values above the design value and therefore an average yearly exceedance rate of 2/3.

4. APPLICATIONS WITH LIMITED AMBIENT DATA

Virtually all of this discussion has focused upon the use of ambient data. Historically, air quality models have been quite useful in providing estimates of air quality levels in the absence of ambient data. The proposed wording of the standard does not preclude the use of such models. As models that provide frequency distributions of air quality are developed their use with the proposed standard will be convenient.

Another potential means of estimating air quality data involves the use of conditional probabilities. While the use of conditional probabilities was discussed earlier in terms of combining different years of data, a more promising use of this technique would involve the construction of historical air quality data sets from relatively short monitoring studies. Very limited ambient data or air quality models may be used to develop frequency distributions for certain types of days or meteorological conditions. Then past historical meteorological data may be used to determine the frequency of occurrence associated with these meteorological conditions. This information may then be combined using conditional probabilities to obtain a general air quality distribution. This particular approach could even be expanded to allow for changes in emissions.

No matter what approach is chosen the two quantities of interest are: (1) the expected number of exceedances per year and (2) the design value, i.e., that concentration with expected number of yearly exceedances equal to 1. However, these modelling and conditional probability constructions may make it possible to assess the risk of violating the standard in the future based upon limited historical data.

5. REFERENCES

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